Tetrahydrophthalic anhydride 85-43-8 | DTXSID3026516

Model Performance

Model	Data
Model	Dala

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.94 days

Global applicability domain: Outside

Local applicability domain index: 4.06e-01

Confidence level: 8.04e-01

Nearest Neighbors from the Training Set

Image not found

Propylbenzene Measured: 24.3 Predicted: 4.02 Image not found

4-Ethyltoluene Measured: 24.3 Predicted: 3.95 Image not found

1,2-Dimethyl-4-ethylbenzene

Measured: 40.7 Predicted: 4.08

Image not found

Tetradeca-1,13-diene Measured: 367 Predicted: 8.69 Image not found

1-Methyl-2-propylbenzene

Measured: 12.5 Predicted: 3.17